Possible critical point in phase diagrams of interlayer Josephson-vortex systems in high-T_c superconductors

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A critical value in the product of the anisotropy parameter and the magnetic field is observed in interlayer Josephson-vortex systems by extensive Monte Carlo simulations. Below/above this critical value the thermodynamic phase transition between the normal and the superconducting states upon temperature sweeping is first/second order. The origin is the intrinsic pinning effect of the layered structure of high-T_c superconductors.

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In the superconducting state, an external magnetic field applied in the Cu-O plane of a high-T_c superconductor induces the so-called Josephson vortices. The center of a Josephson vortex enters into a block layer, the layer between two superconducting Cu-O layers, in order to save the condensation energy of superconductivity [1]. The thermodynamic phase transition and the lattice structure of interlayer Josephson vortices have been attracting considerable interests since the discovery of high-T_c superconductivity. Using a London theory, the structure of Josephson-vortex lattice was derived as the compressed hexagons of triangular lattice pointing along the c axis by Ivlev, Kopnin and Pokrovsky [2]. The interlayer shear modulus was shown to be exponentially small, and the shear deformation of a rhombic lattice might arise through a second-order phase transition. However, at higher temperatures fluctuations are more important, and the London theory is generally inaccurate for discussions about phase transitions. Considerable efforts have been made in order to clarify the thermodynamic phase transition in Josephson-vortex systems both experimentally [3–7] and theoretically [8–12] thereafter. Nevertheless, the understanding for the problem is still not satisfactory yet. Results obtained by different techniques even seem to be contrary to each other. The difficulty in approaching this problem is two-fold. On the experimental side, a small deviation of the direction of the magnetic field from the Cu-O plane can lead to a strong influence of the c-axis component of the magnetic field on thermodynamic properties of the systems, since all the high-T_c superconductors are very anisotropic. On the theoretical side, one has to treat simultaneously anisotropic inter-vortex forces, the commensuration between the vortex alignment and the underlying layered structure, and thermal fluctuations.

In the present Letter, we report new results of extensive Monte Carlo (MC) simulations on the thermodynamic phase transition and the lattice structure of interlayer Josephson vortices. Our results suggest the existence of a critical value of product of the anisotropy parameter and the magnetic field, such that below/above this critical value the thermodynamic phase transition between the normal and the superconducting states is first/second order upon temperature sweeping.

The model Hamiltonian used for the present simulations is the so-called 3D anisotropic, frustrated XY model defined on the simple cubic lattice [13–16]:

$$H = -J \sum_{<i,j>\|x\mathrm{axis}} \cos(\varphi_i - \varphi_j) - J \sum_{<i,j>\|y\mathrm{axis}} \cos(\varphi_i - \varphi_j) - \frac{J}{\gamma^2} \sum_{<i,j>\|\mathrm{caxis}} \cos(\varphi_i - \varphi_j - \frac{2\pi}{\phi_0} \int_i^j A_c dr_c). \qquad (1)$$

Here the y axis is along the external magnetic field, and $\mathbf{y} \perp \mathbf{c} \perp \mathbf{x}$. The unit length of the simple cubic lattice is the distance d between the neighboring Cu-O layers in a cuprate. Therefore, the discreteness in the c axis comes from the underlying layered structure of cuprates, while that in the Cu-O planes is introduced merely for computer simulations. The coupling constant is given by $J = \phi_0^2 d/16\pi^3\lambda_{ab}^2$. The anisotropy parameter is defined by $\gamma = \lambda_c/\lambda_{ab}$, and determines the ratio between the couplings in the Cu-O plane and along the c axis. In the present model, fluctuations in amplitudes of superconducting order parameters and in the magnetic induction are neglected.

Details of simulation technique are summarized as follows: The density of flux lines induced by the external magnetic field is $f = Bd^2/\phi_0$. A Landau gauge is adopted so that $A_x = 0$ and $A_c = -xB$. The system size is $L_x \times L_y \times L_c = 384d \times 200d \times 20d$, which is compatible with the filling factor $f = 1/32$. There are 240 Josephson

flux lines in the ground state. Periodic boundary conditions are applied on phase variables in all directions. A typical simulation process is started from a random configuration of the phase variables at a high temperature, such as $T = 1.5J/k_B$. 30000 and 90000 MC sweeps are used for equilibration and statistics, respectively, at each temperature. The last configuration at a temperature is used as the initial configuration at a slightly lower temperature, where the temperature difference is $\Delta T = 0.1J/k_B$. Around the transition temperature, more than one million MC sweeps are adopted at each temperature, and meanwhile the cooling rate is reduced to $\Delta T = 0.01J/k_B$. Vortices are identified by counting phase differences around plaquettes.

In order to compare our simulation results with existing experimental observations, we choose to study first a system of anisotropy parameter $\gamma = 8$, which is near to that of $YBa_2Cu_3O_{7-\delta}$. The magnetic field corresponding to $f = 1/32$ in our simulations is much stronger than those in experiments, and we come back to this point later. The temperature dependence of the helicity modulus (a quantity proportional to the superfluid density) along the magnetic field and the specific heat is depicted in Fig. 1. There is a clearly observable δ-function like peak in the specific heat at $T_m \simeq 0.96J/k_B$, where the helicity modulus along the direction of magnetic field increase sharply from zero. Shown in the same figure is the temperature dependence of the intensities of Bragg peaks in diffraction patterns at $\mathbf{q}_{xc}^{(1)} = (\pm\pi/8d, 0)$ and $\mathbf{q}_{xc}^{(2)} = (\pm\pi/16d, \pm\pi/d)$. Therefore, a thermodynamic first-order phase transition occurs at T_m, where the gauge symmetry and translation symmetry are broken simultaneously, corresponding to the realization of superconductivity and Josephson-vortex lattice respectively.

The lattice structure of Josephson vortices at low temperatures is shown in Fig. 2. The unit cell is rhombic with short axis along the c direction and of a length of $2d$, and the long axis along the x direction and of a length of $32d$. Josephson vortices are distributed in every block layer for the present parameters $\gamma = 8$ and $f = 1/32$. This structure is the same as that predicted by Ivlev, Kopnin and Pokrovsky [2].

The lattice structure in Fig. 2 is obviously the ground state for $\gamma \geq 8$ when the filling factor is fixed at $f = 1/32$. Therefore we can use it for investigations of thermodynamic properties for large anisotropy parameters by a heating process. The specific heats thus obtained are shown in Fig. 3 for anisotropy parameters $\gamma = 8$, 9, and 10. The δ-function peaks in the curves for $\gamma = 8$ and 9, is suppressed for $\gamma = 10$ [12]. In Fig. 4 we display the temperature and anisotropy parameter dependence of the phase difference between nearest neighboring Cu-O layers $\langle\cos(\varphi_n - \varphi_{n+1})\rangle$. There is a jump in $\langle\cos(\varphi_n - \varphi_{n+1})\rangle$ for $\gamma = 8$ and 9, which is smeared out for $\gamma = 10$. As the jump in $\langle\cos(\varphi_n - \varphi_{n+1})\rangle$ is nothing but the jump in the Josephson energy in units of J/γ^2, there exists a latent heat at the transition temperature for $\gamma = 8$ and 9, but not for $\gamma = 10$, consistently with the data for the specific heat. The value of the latent heat itself is too tiny, about γ^2 times smaller than that in $\langle\cos(\varphi_n - \varphi_{n+1})\rangle$, to be detected directly. On the other hand, from a standard finite-size scaling theory for a first-order phase transition, the height of the δ-function like peak in the specific heat is proportional to the system size [15]. Therefore, by using a large system such as the one in our simulations, the δ-function like peak in the specific heat becomes observable as in Figs. 2 and 3 for the first-order phase transitions.

We have performed simulations for anisotropy parameters $\gamma = 7, 6, \cdots$, down to the isotropic case of $\gamma = 1$ [17]

fixing the filling factor at $f = 1/32$, and observed first-order phase transitions for all these anisotropy parameters. Therefore, the present simulation results indicate that there is a critical anisotropy parameter in between $\gamma = 9$ and $\gamma = 10$ for $f = 1/32$, below/above which the phase transition is first/second order.

Now we look for the reason of the suppression of the first-order phase transition when the anisotropy parameter is increased. Suppose a complete commensuration is achieved between the alignment of the Josephson vortices shown in Fig. 2 and the underlying layered structure of high-T_c cuprates. In other words, the Cu-O layers do not influence the lattice structure of Josephson vortices, but merely fix its position in the c direction. In such a case, the Josephson-vortex lattice should be rescaled into equilateral triangular lattice using the anisotropy parameter γ, and we have a relation as seen in Fig. 5:

$$(2d)^2 = d^2 + (d/2f\gamma)^2,$$

which results in

$$f\gamma = \frac{1}{2\sqrt{3}}. \tag{2}$$

Now we increase the anisotropy parameter from that determined by the above relation when the filling factor f is fixed. Since the repulsive force between Josephson vortices in the c direction is reduced, the Josephson-vortex lattice would be compressed in this direction in order to achieve the energy minimum for the new anisotropy parameter. This reconstruction of Josephson-vortex lattice is forbidden by the underlying layered structure of the high-T_c superconductor. Therefore, the above relation provides a criterion for onset of the intrinsic pinning effect of the layered structure on the formation of Josephson-vortex lattice. For anisotropy parameters larger than that evaluated by the above relation, the lattice structure of Josephson vortices is determined by both the inter-vortex repulsions and the pinning force of the underlying layered structure. The thermodynamic phase transition associated with the formation of the Josephson-vortex lattice can be different in the two regions divided by the above relation.

Numerically, the critical anisotropy parameter for the filling factor $f = 1/32$ is evaluated as $\gamma = 16/\sqrt{3} \simeq 9.24$ by the relation (2). This estimate coincides well with our simulation results, since first-order phase transitions are observed for $\gamma \leq 9$ but not for $\gamma \geq 10$. We have also performed simulations for the filling factor $f = 1/25$, and found the variation of phase transition from first to second order around $\gamma = 8$. This observation is consistent with the relation (2), since for $f = 1/25$ one has the critical anisotropy parameter $\gamma \simeq 7.22$. For $f = 1/36$, we have observed a first-order phase transition even for $\gamma = 10$, consistently with the critical value $\gamma \simeq 10.39$. Namely, our simulation results indicate clearly that the critical anisotropy parameter increases with decreasing filling factor, or magnetic field. Quantitatively, the simple relation (2) seems to give a reasonable estimate on the critical anisotropy parameter.

The same variation of the phase transition should be observed when the anisotropy parameter is fixed while the filling factor, or the strength of the magnetic field, is tuned. The relation (2) can be rewritten as

$$B = \frac{\phi_0}{2\sqrt{3}\gamma d^2}. \tag{3}$$

For $YBa_2Cu_3O_{7-\delta}$ with $\gamma \simeq 8$ and $d = 12\AA$, the critical magnetic field is estimated as $B \simeq 50T$. Therefore the phase transition in the Josephson-vortex systems in $YBa_2Cu_3O_{7-\delta}$ is first order for magnetic fields available experimentally, according to our present study. For $Bi_2Sr_2CaCu_2O_{8+y}$ with $\gamma \simeq 150$ and $d = 15\AA$, the critical magnetic field is evaluated as $B \simeq 1.7T$, which can be checked experimentally.

The phase transition of interlayer Josephson vortices in a layered superconductor has been addressed theoretically by Blatter, Ivlev and Rhyner [8] and Balents and Nelson [11]. In these theories, the Josephson-vortex lattice melts in-between the layers with the formation of a smectic-like vortex liquid, via a second-order phase transition (see also [2]). Therefore, for strong magnetic fields the theories give a reasonable scenario for the phenomena in Josephson-vortex systems observed in the present simulations.

The importance of thermal fluctuations in the phase transition should be stressed. For example, about one vortex-antivortex pair is thermally excited per Josephson flux at each xc section at $T = 0.8J/k_B$, a temperature lower than the corresponding transition point, for $\gamma = 8$ and $f = 1/32$ [18]. Energetically, an additional Josephson vortex only costs energy of order of J/γ^2, which becomes very small when the anisotropy parameter γ is large [19]. Most of the thermally excited Josephson vortices and antivortices are confined in same block layers and form overhangs in flux lines, or closed loops. As the result, for large anisotropy parameters Josephson flux lines induced by the magnetic field collide with each other in same block layers even below the transition temperature [18]. Therefore, these thermally excited Josephson vortices and antivortices play important roles in smearing out the first-order phase transition in a Josephson-vortex system in a layered superconductor with a large anisotropy parameter [9,20].

In summary, from extensive Monte Carlo simulations we have found a critical value in the product of the anisotropy parameter and magnetic field in interlayer Josephson-vortex systems in high-T_c superconductors. Below/above this critical value, the thermodynamic phase transition between the normal state and the superconducting state is first/second order. According to the present results, the phase transition in Josephson-vortex systems in $YBa_2Cu_3O_{7-\delta}$ is first order under magnetic fields up to $B \simeq 50T$, while it varies from first to second order in $Bi_2Sr_2CaCu_2O_{8+y}$ as the magnetic field is increased to across $B \simeq 1.7T$.

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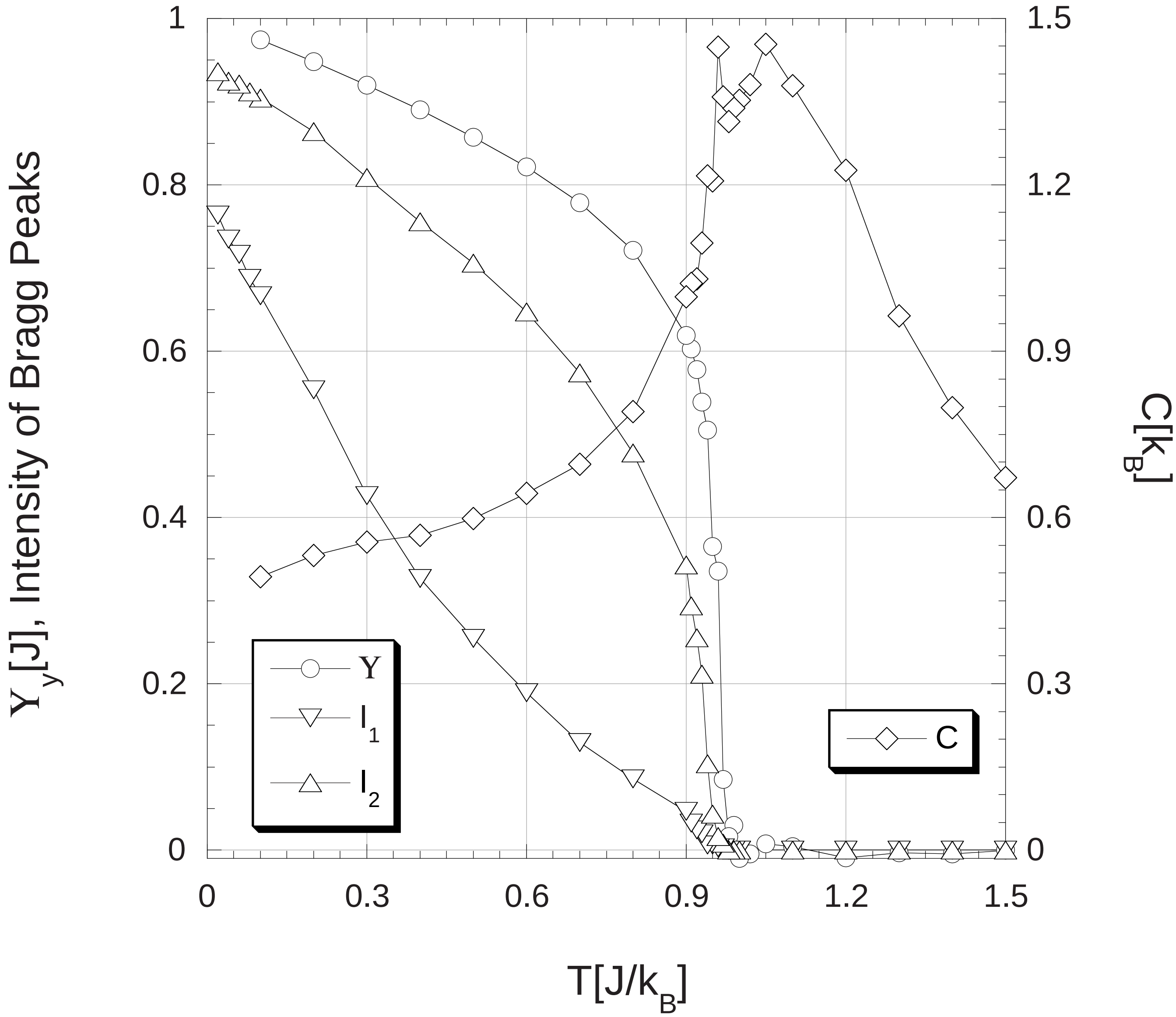
Fig. 1: Temperature dependence of the helicity modulus along the magnetic field, the specific heat and the intensities I_1 and I_2 for the Bragg peaks at $\mathbf{q}_{xc}^{(1)} = (\pm\pi/8d, 0)$ and $\mathbf{q}_{xc}^{(2)} = (\pm\pi/16d, \pm\pi/d)$ respectively for $\gamma = 8$ and $f = 1/32$.

Fig. 2: Josephson vortex lattice for $\gamma = 8$ and $f = 1/32$ obtained by MC simulations of a cooling process from a random state at high temperatures.

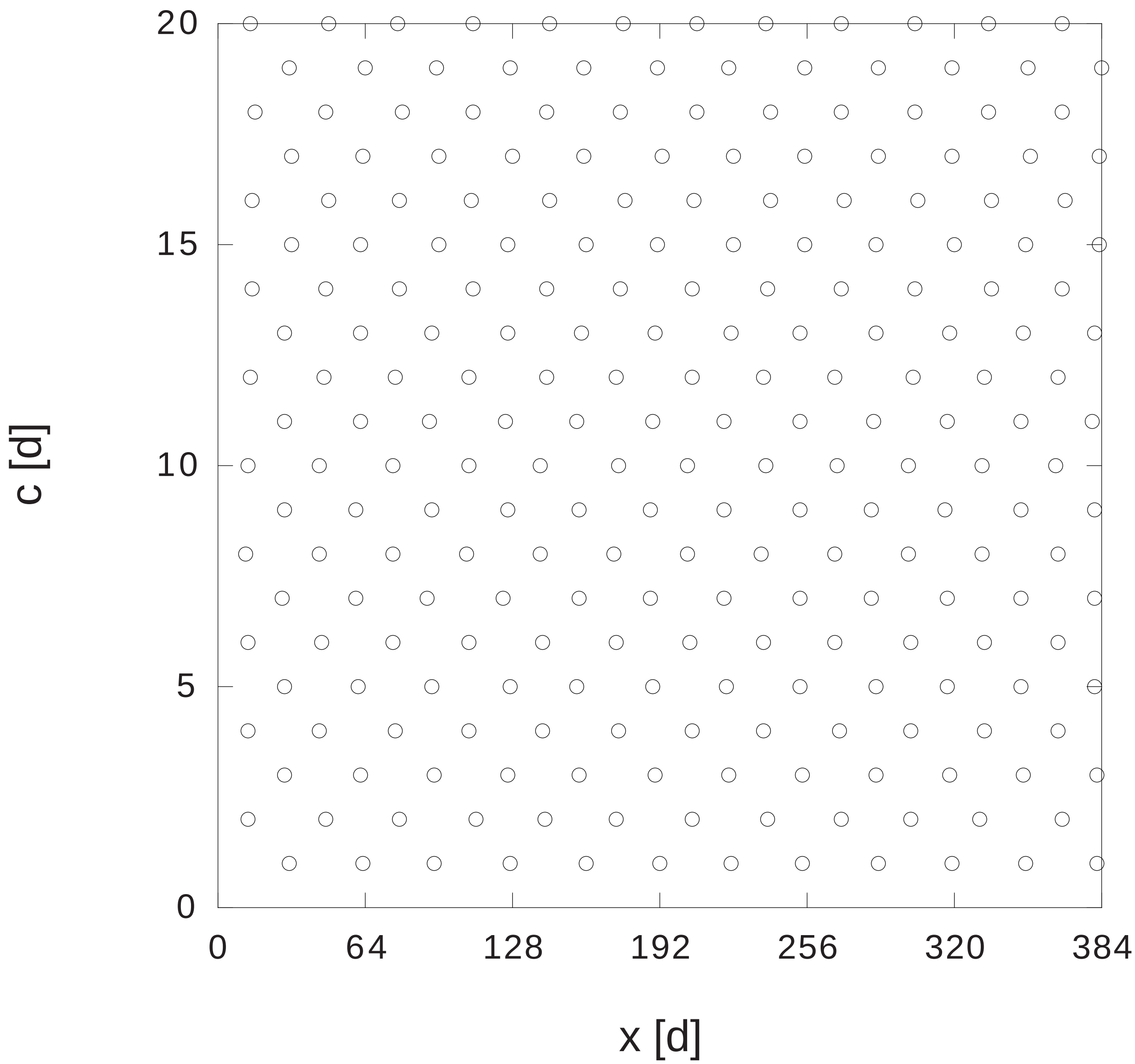
Fig. 3: Temperature dependence of the specific heat for $\gamma = 8$, 9 and 10 and $f = 1/32$. Data for $\gamma = 8$ and 9 are shifted by constants.

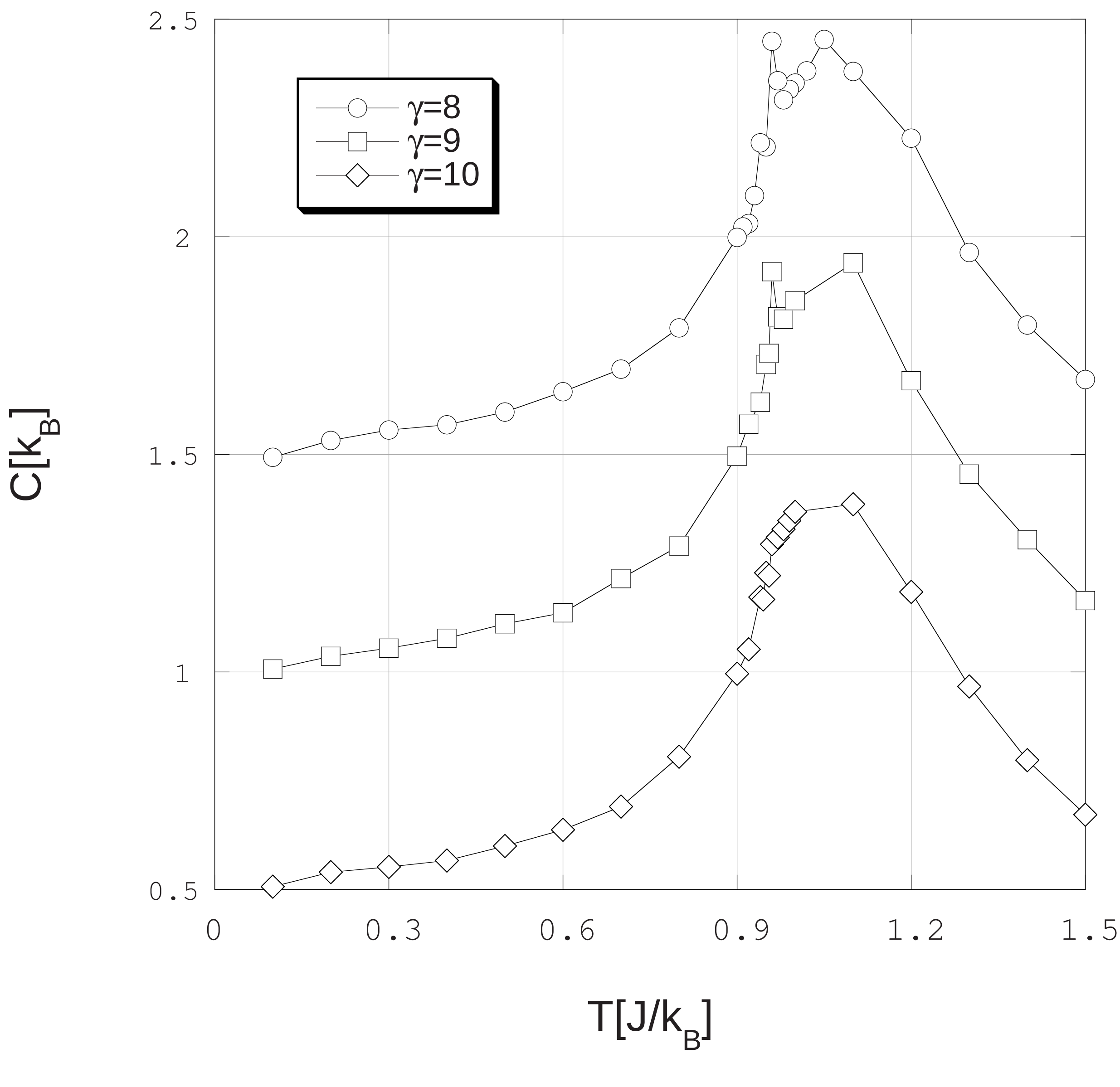
Fig. 4: Temperature dependence of the phase difference between nearest neighboring Cu-O layers for $f = 1/32$. The lines are for eye-guide.

Fig. 5: Real-space unit cell of the Josephson-vortex lattice in a layered superconductor of a large anisotropy parameter.

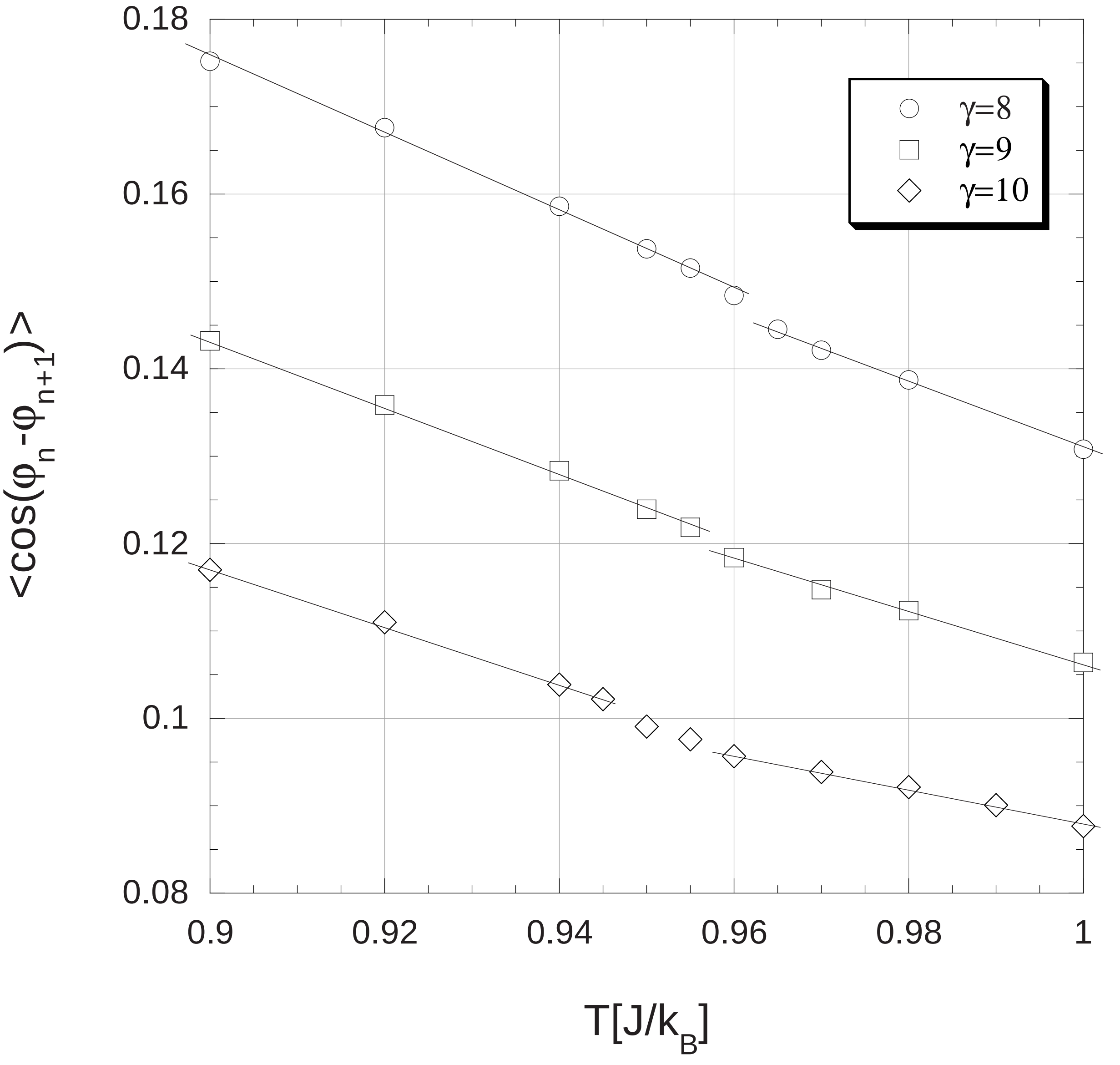


1
0.8
0.6
0.4
0.2
0
1.5
1.2
0.9
0.6
0.3
0
0
0.3
0.6
0.9
1.2
1.5
Y_y[J], Intensity of Bragg Peaks
C[k_B]
T[J/k_B]
Y
I_1
I_2
C

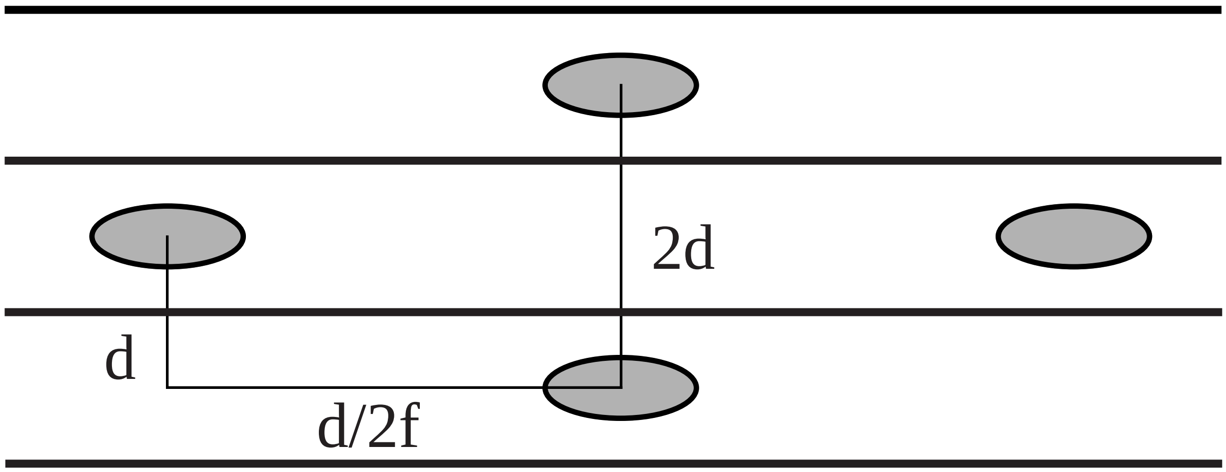

20
15
10
5
0
0
64
128
192
256
320
384
x [d]
c [d]



γ=8
γ=9
γ=10
2.5
2
1.5
1
0.5
0
0.3
0.6
0.9
1.2
1.5
C[k_B]
T[J/k_B]



0.18
0.16
0.14
0.12
0.1
0.08
0.9
0.92
0.94
0.96
0.98
1
$<\cos(\varphi_n-\varphi_{n+1})>$
$T[J/k_B]$
γ=8
γ=9
γ=10


2d
d
d/2f